

POLARIZATION AND SPACE CHARGE
EFFECTS IN ELECTRODE DESIGN

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Summary

Electrostatic field effects in high pressure discharges which provide physical insight into the problem of electrode design are derived. The coupled set of charge transport equations and Poisson's equation have been analytically studied using perturbation theory techniques. Our study reveals that the homogeneous field must be supplemented by the inhomogeneous contributions of space charge and polarization effects which arise from nonuniform plasma ionization and local nonconservation of each species current. The validity of a commonly used boundary condition is examined and found untenable. Implications for the computational design of electrodes are presented.

Introduction

The rational engineering design of electrodes for externally ionized as well as self-sustained glow discharges requires an appreciation of dominant physical effects as well as mathematical consequences of the modelling equations. Contemporary design practice invokes techniques which vary in sophistication from the widely used empirical method of cut and try to numerical methods of solving the nonlinear Poisson equation in arbitrary materials and geometries.

To some investigators, a very appealing feature of discharge physics is its insatiable appetite for computationally recondite theories which must of course be self-consistently linked together. Unfortunately, in our haste to compute, we sometimes lose sight of the most elementary issues which can then sabotage us from undergrowth of arcanna in which they hide. Such a problem in electrode design and in calculations of the discharge field is how to prescribe the boundary conditions of the field. In tackling this problem, which is addressed below, we have begun with a fresh look at the electrostatics of discharges based on elementary undergraduate considerations. Our conclusions have provided us with intuitive insight into the physical mechanisms which govern the field behavior and have guided us in the construction of our computational models used in electrode design.

In the following, we limit ourselves to the design of two dimensional electrode profiles. In practice, an approximate solution to the real problem of determining a three dimensional profile may be obtained by smoothly fitting together rectilinear and axisymmetric profiles. Theoretical work is in progress to address the computational problem of a self-consistent three dimensional electrode design.

Historical Survey

The Zeoroeth Order and most prevalent method of contemporary electrode design assumes that the field is completely homogeneous and a resort is made to the conformal mapping solutions of Laplace's equation which appear in Maxwell's treatise. The algorithm for design was worked out by Rogowski and appears in Cobine's book.¹ The Rogowski profile results from a semi-infinite cartesian coordinate system. The correct solution for a finite width contour is in principle available but contains implicit functions of the elliptic functions of the first and second kind.² The Chang profile results from analytically continuing the Rogowski profile and requiring maximal uniformity of the field on the center of the electrode.³ In addition to these analytic techniques, rather elaborate computer codes now exist to solve Laplace's equations in arbitrary materials and subject to standard mixed boundary conditions on a finite enclosing surface.

The objective of these analytical techniques is to produce an electrode profile on which the field intensity is maximally uniform and monotonically decreasing from the symmetry plane of the profile. However theoretical and experimental evidence strongly suggests that this may not be the most desirable engineering criterion. In ref 4 investigations are reported in which the electrode profile was shaped to provide for abrupt deviations of the field from the above conditions near the edge of the discharge. The result was a reduction of discharge constriction, a very sharp discharge edge and very flat optical uniformity. Furthermore it is a commonly observed fact that large discharge devices tend to arc in preferential locations on the electrodes. These locations are usually found where one can intuitively perceive the existence of large field stress concentrations. Thus in such cases device failure is due to a local weakness in design and not a global deficiency. A highly desirable engineering design objective is then to distribute such local stresses throughout a larger area to improve uniformity of performance throughout the device.

There are two issues which are raised by the above techniques. A major limitation of the analytic techniques and of a standard "Laplace" computer code is that they are normally limited in validity to rectilinear coordinate systems with translational symmetry in the third dimension and thus may not be casually applied to cylindrical geometries which are essential to switch design. The solutions derived from conformal mapping techniques may not be applied to cylindrical geometries because the applicable part of the cylindrical Laplacian is not harmonic in the sense of complex variable theory. The "Laplace" code

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solutions on the other hand do not in general use the cylindrical Laplacian for the numerical development. Thus an uncritical use of standard profiles in cylindrical devices which involve a mere rotation of a rectilinear solution about the symmetry axis is unwarranted. Work is now in progress to develop standard techniques for this problem.

The second major limitation which comes to light in a practical application of the numerical technique is that a real device geometry may occasionally possess a boundary which is sufficiently distant from the cavity that it sets up an asymptotic boundary condition. In practice the investigator may then impose an artificial boundary on the device which approximates the asymptotic consequences in a bounded region. However, even though this artificial condition may in some sense be a good overall approximation to the true field behavior, it can introduce distortions to the fringing field behavior and hence to the roll-off contour of an electrode profile. A better practical approximation to the problem of distant boundaries is to impose the true asymptotic conditions in a finite domain which has been mapped from the "infinite" domain. The technique of numerical mapping as it is addressed in the following companion paper thus retains the essential fringing field behavior characteristics of the conformal mapping solutions.

The technique of merely solving Laplace's equation for electrode design works well in self-sustained discharges.⁴ However, as we will show below, inhomogeneous source terms do not completely disappear for this case, they are only less important than those in the externally sustained case.

In externally sustained discharges, the spatially non-uniform primary ionization causes the cavity field to deviate substantially from the homogeneous field. Instead of solving Laplace's equation, a nonlinear Poisson equation, resulting from current conservation requirements, is solved numerically.⁵⁻⁸ In our analysis we will investigate assumptions which enter into this procedure. We will find that the assumption of vanishing normal field at the edge of a discharge confinement region is not merely invalid as would be generally suspected, but that it is also entirely wrong and misleading.⁵⁻⁷ Next we will investigate the assumption of electron drift current conservation which leads to the applicable nonlinear Poisson equation. We will discover nonconservation of electron drift current with a consequent space charge and second order field distortion.

Analysis

We will derive our higher order effects from the coupled set of equations for electron and ion transport together with Poisson's equation.

$$\frac{\partial n_e}{\partial t} + \vec{\nabla} \cdot n_e \vec{v} = S - \alpha n_i n_e + \beta n_e$$

$$\frac{\partial n_i}{\partial t} + \vec{\nabla} \cdot n_i \vec{v}_i = S - \alpha n_i n_e + \beta n_e$$

$$\vec{\nabla}^2 \phi = - \frac{e}{\epsilon_0} (n_i - n_e)$$

Here $n_{i,e}(\vec{x})$ is the number density of ions or electrons. $v_{i,e}(E/N)$ is the drift velocity due to the neutral gas, N , and the normalized electric field, $\vec{E}(\vec{x}) = -\vec{\nabla} \phi$. The recombination rate is $\alpha(E/N)$ and the combined secondary ionization and attachment rate is $\beta(E/N)$. The spatially varying primary ionization source term, $S(\vec{x})$, is also an implicit function of $\vec{E}(\vec{x})$ and $\vec{B}(\vec{x})$. But we neglect the self-consistent coupling of S to E and B for this analysis. In the event that S is provided for by an electron beam, then the fast primary electrons will eventually be thermalized by the discharge gas and will contribute to the space charge term. This can be a substantial effect, but we will neglect it here for the sake of clarity in our following arguments. For the sake of algebraic simplicity we simplify our considerations to the case of $\beta=0$. Analogous conclusions may be drawn from an extension of our analysis to the case of $\beta \neq 0$. We have neglected the diffusion current and its derivatives in comparison to the convection current and its derivatives for the specialized case of high pressures.

The conventional procedure is to assume:

- Steady state, $\frac{\partial n_{i,e}}{\partial t} = 0$
- Quasi-neutrality, $n_i = n_e$, for all \vec{x} ; and
- Separate species current conservation, $\vec{\nabla} \cdot n_e \vec{v}_e = 0 = \vec{\nabla} \cdot n_i \vec{v}_i$

From the electron current equation, for example, we then obtain $n_e = \sqrt{S/\alpha}$, which together with current conservation yields a nonlinear conductivity equation:

$$\vec{j}_0 = \sigma(\vec{E}, \vec{x}) \vec{E} = \left\{ \sqrt{\frac{S}{\alpha}} \frac{v_e}{E} \right\} \vec{E}.$$

This further results in the nonlinear Poisson equation:

$$\vec{\nabla}^2 \phi = \vec{E} \cdot \vec{\nabla} \ln \left\{ \sqrt{\frac{S}{\alpha}} \frac{v_{i,e}(E/N)}{\sqrt{\alpha(E/N)}} \right\}.$$

Here $v_{i,e}(E/N)$ and $\alpha(E/N)$ are known either experimentally or by kinetic calculations. The nonlinear Poisson equation is then solved subject to appropriate boundary conditions to give a First-Order solution to the discharge field problem.

In the case of a self-sustained discharge, the external ionizing term, $S(\vec{x})$, disappears and must be

replaced by the combined secondary ionization and attachment term in . We then obtain $n_{i,e} = \beta/\alpha$ which upon inserting into the current conservation equation and applying the chain rule yields:

$$\frac{\partial}{\partial E} \left\{ \frac{\beta(E/N) v_{i,e}(E/N)}{E \alpha(E/N)} \right\} \vec{\nabla} \cdot \vec{E} = 0$$

Which results in Laplace's equation for the field, $\nabla^2 \phi = 0$.

Thus the First-Order development of the coupled set of equations for a self-sustained discharge results in a homogeneous electric field. Therefore electrodes for this case may be based on a harmonic analysis as has been the practice.

In the following we challenge an assumption which is often and recklessly made.²⁻⁵ Namely that the electric field normal to a discharge confinement wall vanishes. This assumption is equivalent to assuming that the fringing fields which occur with any bounded conductor in free space are contained by the confined plasma "since the plasma is a conductor." Another argument one may occasionally encounter which supports the idea of confined field lines in the plasma is that the plasma is so strongly polarized that it traps the field lines by dielectric focusing as in the optical phenomenon of total internal reflection. We will analyze both points of view and demonstrate that the assertion of a vanishing normal component of the field is insupportable and spurious.

Space Charge Effects From Current Conservation

For convenience, we model α and v_e as power functions of E/N and assume that N is constant.⁷ That is we neglect gasdynamic effects.

Let $\alpha = A^2 E^{-2a}$ and $v_e = B E^b$

and define $s(x) = \frac{S(x)}{S(0)}$ and $\zeta = \frac{1}{2(a+b)}$

Then the space charge density is:

$$\rho = \epsilon_0 \vec{\nabla} \cdot \vec{E} = -\epsilon_0 \zeta \vec{E} \cdot \vec{\nabla} \ln[s(x)].$$

Now from $j_0 \approx j_e = en_e v_e = e\sqrt{S} \frac{B}{A} E^{a+b}$

and $V_0 = - \int_0^{\ell} \vec{E} \cdot d\vec{\ell}$, we obtain

$$E(x) = -V_0 \frac{[s(x)]^{-\zeta}}{\int_0^{\ell} [s(x)]^{-\zeta} d\ell}$$

and thus

$$\rho = -\epsilon_0 V_0 \frac{\vec{\nabla} E [s(x)]^{-\zeta}}{\int_0^{\ell} [s(x)]^{-\zeta} d\ell}.$$

The charge stored within a stream tube between electrodes is thus

$$Q = \epsilon_0 V_0 \left\{ \frac{[s(\ell)]^{-\zeta} - [s(0)]^{-\zeta}}{\int_0^{\ell} [s(x)]^{-\zeta} d\ell} \right\}$$

Using the definition of capacitance per unit area $C/A = (Q/A)/V$ we find that the ratio of the capacitance of the discharge to that of the free space capacitor is given by the term in braces. For a uniform source we see that the ratio vanishes. For a very severe case, we may approximate $s(x) \approx \exp(-kx)$. This corresponds to a real AFWL device, PULSAR, where $k = -0.216$, $a = 0.78$, $b = 0.56$. We obtain the ratio of the capacitance of a flux tube to that of the free space capacitor plates to be $C_{dis}/C_0 = \mu = 0.081$. That is the free space capacitor contributes over 90% of the field behavior to the device and hence the field is mostly homogeneous and mostly fringes at its edges.

We pause to note, however, that even though the bulk effect of the discharge on the overall capacitance is small, the local field intensity may deviate substantially from the homogeneous field. In the case of PULSAR we have ($\ell = 5$):

$$\frac{E(x)}{E_0} = \frac{\mu \ell}{e^{\mu \ell} - 1} e^{\mu x} \uparrow_{0.80}^{1.20} \text{ as } x \uparrow_0^{\ell}.$$

Polarization Effects for Current Conservation

Since we now know that the discharge stores charge in the bulk we would like to know how it behaves in small localities. In a differential volume of cross sectional area dA and length dx along a flux line we have a charge dQ and a voltage drop $dV = Edx$. Together these lead to an incremental capacitance per unit area of

$$C' = \frac{dQ/dA}{dV} = \frac{\rho}{E} \frac{dx}{dx} = \epsilon_0 \zeta \vec{E} \cdot \vec{\nabla} \ln [s(x)]$$

We thus see that our externally ionized discharge can store charge and possesses an incremental capacitance due to its non-uniform conductivity. We will now outline a calculation of the discharge's associated equivalent relative permittivity on the basis of electrostatic energy arguments. We have

$$U = 1/2 \epsilon_0 E^2 = 1/2 \epsilon_0 E_o^2 \left\{ \left[\frac{\ell [s(x)]^{-\zeta}}{\int_0^\ell [s(x)]^{-\zeta} d\ell} \right]^2 \right\}$$

$$= 1/2 \epsilon_{rel} \epsilon_0 E_o^2$$

The term in braces is thus an equivalent relative local dielectric constant of the discharge in the sense of indicating either constriction or dilation of the field lines in the transverse direction as Faraday's rubber lines of force would tend towards. For the case of PULSAR,

$$\epsilon_{rel}(x) = \left[\frac{\mu \ell}{e^{\mu \ell - 1}} e^{\mu x} \right]^2 \int_{0.65}^{1.50} \text{ as } x \int_0^\ell .$$

Although we are presenting an exaggerated and pathological case we can clearly see the general trends. The discharge acts like a dielectric lens which bends the fringing field lines away from the cavity near the cathode and towards the cavity near the anode. This explains the empirically determined engineering practice of sharply rounding cathode roll-off contours and mildly rounding anode roll-off contours when the e-beam is injected from the cathode side.

Once again we see that the discharge only slightly affects the true field in comparison to the homogeneous field (although significantly for electrode design purposes). Thus in the vicinity of the discharge edge we are completely unjustified in asserting that the normal electric field component vanishes as is done in ref 5-7. The effect of imposing this artificial condition is to distort the curvature of the potential surfaces near the roll-off thus invalidating any electrode profile design accomplished in this manner. In order to retain the correct field behavior near the roll-off we must correctly match the field behavior in the asymptotic region. This is best

accomplished by the mapping techniques presented in the following companion paper.

A second consequence of the smallness of the distortions introduced by the polarization of the discharge is that we must now include all surrounding dielectrics in our calculations.

Nonconservation of Species Currents

In this section we outline an investigation into the validity of assuming conservation of each species current. Unfortunately the lengthy and tedious algebra involved mandates a condensation of our reasoning into its most salient features. We will find that each species current is not independently conserved and that as a result the true field will vary from the first order field by Second-Order effects due to power loading.

First we note that in deriving our non-linear Poisson equation, that we could just as easily have used v_i as v_e . However the dependence of v_e on E/n varies widely among gases with a power dependence varying from $b = 0.5$ for CO_2 to $b = 0.9$ for N_2 whereas for most bases the power for v_i is very close to unity. We are thus led to seek out disparities in the overall behavior due to this difference.

$$\text{Let } v_e = BE^b \text{ and } v_i = CE^c$$

then

$$\frac{j_i}{j_e} = \left(\frac{1}{1-\delta} \right) \frac{C}{B} E^{c-b}$$

where

$$\delta \equiv \frac{\eta_i - \eta_e}{\eta_i}$$

For the pathological case of PULSAR we have $\delta \ll 10^{-3}$

and $\delta' \approx k \delta \ll 10^{-3}$. We may thus neglect δ in our subsequent remarks, although in general δ must be retained throughout all manipulations to ensure that correct perturbation orders are addressed.

From $j_i + j_e = j_o$, we obtain

$$\frac{j_i}{j_o} = \frac{\frac{C}{B} E^{c-b}}{1 + \frac{C}{B} E^{c-b}}$$

$$\frac{j_e}{j_o} = \frac{1}{1 + \frac{C}{B} E^{c-b}}$$

In the spirit of successive approximations we thus see that $\vec{\nabla} \cdot \vec{j}_{i,e} = 0$ implies $|\vec{\nabla} \cdot \vec{E}| > 0$ which in the next higher order treatment implies that $|\vec{\nabla} \cdot \vec{j}_{i,e}| > 0$.

Using E in terms of j_i/j_o from above, we may rewrite $\alpha(E)$ and $v_{i,e}$ and thus $n_{i,e}$ in terms of j_i/j_o . Thus the ion current conservation equation may be cast into a form which depends only on j_i/j_o and auxiliary parameters:

$$\vec{\nabla} \cdot \vec{j}_i = eS - e \left\{ \left(\frac{j_o}{e} - \frac{A}{C} \right)^2 \left(\frac{C}{B} \right)^\theta \right\} \left(\frac{j_i}{j_o} \right)^{-\eta} \left[1 - \left(\frac{j_i}{j_o} \right) \right]^\theta$$

$$\text{where } \eta = 2 - \frac{a+b}{c-b} \text{ and } \theta = 2 - \frac{a+c}{c-b}.$$

We have analytically investigated this equation with perturbation theoretic techniques based on the assumption of a slowly varying $j_i(x)$ and using linearization wherever possible due to the smallness of j_i/j_o .

For $\vec{\nabla} \cdot \vec{j}_i \approx 0$ and $j_i/j_o \ll 1$ we set

$$\frac{j_i(x)}{j_o} = [S(x)]^{-1/\eta} [1 + \epsilon(x)]$$

where $\epsilon(x)$ is the perturbing term. Inserting this into our last expression for current conservation and applying the above techniques we obtain

$$E(x) \sim [s(x)]^{-\zeta} \left\{ 1 + \frac{1}{2a+b+c} \left[\exp \left(\frac{\theta}{2} \int_0^x S(x) dx \right) - 1 \right] \right\}$$

The term in braces depends on the factor $\frac{e}{j_o} \int_0^x S(x) dx$ which is approximately $\int n_e dx / v_e$ which increases with power loading for a relatively fixed E . Thus the first order electric field solution due to current conservation deviates from the true solution by a small term dependent on the local power loading. For a case where $S(x)$ is constant and yields $n_e \approx 10^{12}$ with PULSAR like parameters, we see that the first order variation vanishes and the second order term contributes a 10 percent variation to the field intensity and a 20 percent variation to the

permittivity. Thus this power loading induced space charge effect cannot in general be ignored.

Having established the effect of species current non-conservation on the discharge we have now justified the need to solve the fully coupled set of transport equations together with Poisson's equation in order to correctly determine the electric field for electrode design for externally ionized discharges. This aspect of the general problem is currently being pursued with a mid-term priority.

Finally, we may note that even if we set $S(x)=0$ in our rewritten ion conservation equation, that j_i/j_o will still have a spatial dependence (we of course must add the β term which we dropped earlier). Thus to second order, even self-sustained discharges will possess electric fields which deviate from the homogeneous solution.

Conclusion

The electric field of an externally ionized discharge is mostly homogeneous. Space charge can affect the local field intensity by as much as 20 percent in severe cases. Discharge polarization can enhance or diminish transverse field structure, i.e., fringing, by as much as 50 percent. A rational electrode design theory must predict these effects.

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